

Ethane
74-84-0 | DTXSID6026377

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 3.26 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.76e-01

Confidence level: 7.67e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethanol</div> <div>Measured: 1.58</div> <div>Predicted: 2.24</div>	<div>Image not found</div> <div>Methanol</div> <div>Measured: 2.75</div> <div>Predicted: 2.76</div>	<div>Image not found</div> <div>1-Propanol</div> <div>Measured: 3.02</div> <div>Predicted: 4.69</div>
<div>Image not found</div> <div>Ethyleneimine</div> <div>Measured: 6.03</div> <div>Predicted: 4.17</div>	<div>Image not found</div> <div>Thioacetamide</div> <div>Measured: 6.03</div> <div>Predicted: 6.43</div>	